



chain nodes :

7 14 15 16 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42
 43 44 45 46 47 48 49 64 65 69 73 75 80 84 88 89 90 91 92 93 94 95 96 97
 98 99 100 101 102 103 104 118 119 120 121 122 123 124

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 17 18 19 20 21 22 50 51 52 53 54 55 56 57
 58 59 60 61 62 63 66 67 68 70 71 72 74 76 77 78 79 81 82 83 85 86 87 105
 106 107 108 109 110 111 112 113 114 115 116 117

chain bonds :

4-7 7-8 9-16 10-15 11-14 12-26 16-22 18-23 19-24 20-25 26-124 27-28 29-30 32-33
 32-34 35-36 35-37 38-39 38-40 41-42 41-43 44-45 44-46 47-48 47-49 57-64 61-65
 68-69 70-101 72-73 74-75 78-80 82-123 83-84 86-92 87-88 88-89 89-90 89-91 90-94
 90-98 92-93 94-95 95-96 95-97 98-99 98-100 101-102 102-103 102-104 108-120 112-121
 114-122 117-118 118-119

ring bonds :

1-2 1-6 1-66 2-3 3-4 3-51 4-5 5-6 5-50 8-9 8-13 9-10 10-11 11-12 12-13 17-18
 17-22 18-19 19-20 20-21 21-22 50-60 51-56 52-53 52-57 53-54 53-82 54-55 55-56
 56-57 58-59 58-63 59-60 60-61 61-62 62-63 63-86 66-67 66-74 67-68 68-70 70-71
 71-72 72-87 74-76 76-77 77-78 77-105 78-79 79-81 81-82 81-83 83-85 85-117 86-87
 105-106 105-110 106-107 107-108 108-109 109-110 109-111 111-112 111-116 112-113
 113-114 114-115 115-116 116-117

exact/norm bonds :

1-66 3-51 4-7 5-50 7-8 8-9 8-13 9-10 9-16 10-11 10-15 11-12 11-14 12-13 16-22
 17-18 17-22 18-19 19-20 19-24 20-21 20-25 21-22 26-124 27-28 29-30 32-33 32-34
 35-36 35-37 38-39 38-40 41-42 41-43 44-45 44-46 47-48 47-49 50-60 51-56 53-82
 63-86 66-67 66-74 67-68 68-69 68-70 70-71 71-72 72-73 72-87 74-75 74-76 76-77
 77-78 77-105 78-79 78-80 79-81 81-82 81-83 82-123 83-85 83-84 85-117 86-87 86-92
 87-88 88-89 89-91 90-98 102-103 102-104 108-120 109-111 112-121 114-122 116-117
 118-119

exact bonds :

12-26 18-23 57-64 61-65 70-101 89-90 90-94 92-93 94-95 95-96 95-97 98-99 98-100
 101-102 117-118

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 52-53 52-57 53-54 54-55 55-56 56-57 58-59 58-63 59-60
 60-61 61-62 62-63 105-106 105-110 106-107 107-108 108-109 109-110 111-112 111-116
 112-113

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS
49:CLASS 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:CLASS 65:CLASS 66:Atom 67:Atom 68:Atom
69:CLASS 70:Atom 71:Atom 72:Atom 73:CLASS 74:Atom 75:CLASS 76:Atom 77:Atom 78:Atom
79:Atom 80:CLASS 81:Atom 82:Atom 83:Atom 84:CLASS 85:Atom 86:Atom 87:Atom 88:CLASS
89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 95:CLASS 96:CLASS 97:CLASS
98:CLASS 99:CLASS 100:CLASS 101:CLASS 102:CLASS 103:CLASS 104:CLASS 105:Atom 106:Atom
107:Atom 108:Atom 109:Atom 110:Atom 111:Atom 112:Atom 113:Atom 114:Atom 115:Atom
116:Atom 117:Atom 118:CLASS 119:CLASS 120:CLASS 121:CLASS 122:CLASS 123:CLASS 124:CLASS